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```
Welcome to STN International
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NEWS
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                 New pricing for the Save Answers for SciFinder Wizard within
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         SEP 01
                 STN Express with Discover!
                 KOREAPAT now available on STN
NEWS
         OCT 28
        NOV 30
                 PHAR reloaded with additional data
NEWS
NEWS
      6
        DEC 01
                 LISA now available on STN
      7
         DEC 09
                 12 databases to be removed from STN on December 31, 2004
NEWS
                MEDLINE update schedule for December 2004
NEWS
      8 DEC 15
     9 DEC 17
                ELCOM reloaded; updating to resume; current-awareness
NEWS
                 alerts (SDIs) affected
                 COMPUAB reloaded; updating to resume; current-awareness
NEWS
     10 DEC 17
                 alerts (SDIs) affected
                 SOLIDSTATE reloaded; updating to resume; current-awareness
NEWS
     11 DEC 17
                 alerts (SDIs) affected
                 CERAB reloaded; updating to resume; current-awareness
     12 DEC 17
NEWS
                 alerts (SDIs) affected
                 THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
     13 DEC 17
NEWS
     14 DEC 30
                EPFULL: New patent full text database to be available on STN
NEWS
     15 DEC 30
                CAPLUS - PATENT COVERAGE EXPANDED
NEWS
                 No connect-hour charges in EPFULL during January and
     16 JAN 03
NEWS
                 February 2005
                 CA/CAPLUS - Expanded patent coverage to include Russia
NEWS
     17 JAN 11
                 (Federal Institute of Industrial Property)
```

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

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FILE 'HOME' ENTERED AT 09:23:39 ON 24 JAN 2005

=>

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
8.19 8.19

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 09:46:46 ON 24 JAN 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 JAN 2005 HIGHEST RN 819046-01-0 DICTIONARY FILE UPDATES: 23 JAN 2005 HIGHEST RN 819046-01-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\STNEXP4\QUERIES\awl.str

L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT * Structure attributes must be viewed using STN Express query preparation.

Uploading C:\STNEXP4\QUERIES\aw2.str

L2 STRUCTURE UPLOADED

=> Uploading C:\STNEXP4\QUERIES\aw3.str

L3 STRUCTURE UPLOADED

Page 2

=> .

=> s 11SAMPLE SEARCH INITIATED 09:50:24 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 61448 TO ITERATE 1.6% PROCESSED 1000 ITERATIONS 0 ANSWERS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 FULL FILE PROJECTIONS: ONLINE **INCOMPLETE** BATCH **INCOMPLETE** EXCEEDS 1000000 PROJECTED ITERATIONS: PROJECTED ANSWERS: EXCEEDS L40 SEA SSS SAM L1 => => Uploading C:\STNEXP4\QUERIES\aw4.str STRUCTURE UPLOADED L5 => s 15SAMPLE SEARCH INITIATED 10:09:23 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 34843 TO ITERATE 0 ANSWERS 2.9% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 FULL FILE PROJECTIONS: ONLINE **INCOMPLETE** BATCH **INCOMPLETE** PROJECTED ITERATIONS: 685710 TO 708010 O TO PROJECTED ANSWERS: 0 SEA SSS SAM L5 L6 Uploading C:\STNEXP4\QUERIES\aw5.str STRUCTURE UPLOADED L7 => s 17SAMPLE SEARCH INITIATED 10:13:06 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 49340 TO ITERATE 0 ANSWERS 2.0% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 FULL FILE PROJECTIONS: ONLINE **INCOMPLETE** BATCH **INCOMPLETE** PROJECTED ITERATIONS: 973556 TO 1000044 O TO PROJECTED ANSWERS: L8 0 SEA SSS SAM L7

Uploading C:\STNEXP4\QUERIES\aw6.str

STRUCTURE UPLOADED

0 SEA SSS SAM L13

PROJECTED ITERATIONS: PROJECTED ANSWERS: 0 TO

198224 TO 210336

BATCH **COMPLETE**

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

=> s 113SAMPLE SEARCH INITIATED 10:21:19 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 10214 TO ITERATE

1000 ITERATIONS

=> Uploading C:\STNEXP4\QUERIES\aw8.str

STRUCTURE UPLOADED

9.8% PROCESSED

0 SEA SSS SAM L11 L12

PROJECTED ANSWERS: OTO

BATCH **COMPLETE** 92570 TO 100910 PROJECTED ITERATIONS:

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

20.7% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

0 ANSWERS

0 ANSWERS

=> s 111 SAMPLE SEARCH INITIATED 10:20:07 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 4837 TO ITERATE

=> Uploading C:\STNEXP4\QUERIES\aw7.str

=>

STRUCTURE UPLOADED

0 SEA SSS SAM L9

PROJECTED ANSWERS: O TO

BATCH **INCOMPLETE** PROJECTED ITERATIONS: 922223 TO 948017

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

2.1% PROCESSED 1000 ITERATIONS 0 ANSWERS

=> s 19SAMPLE SEARCH INITIATED 10:18:52 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 46756 TO ITERATE

L9

L11

L13

Page 4

=> search 111
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 10:21:32 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 96489 TO ITERATE

100.0% PROCESSED 96489 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.14

L15 0 SEA SSS FUL L11

=> search 113
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 10:22:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 203759 TO ITERATE

100.0% PROCESSED 203759 ITERATIONS SEARCH TIME: 00.00.13

0 ANSWERS

L16 0 SEA SSS FUL L13

=> Uploading C:\STNEXP4\QUERIES\aw10.str

L17 STRUCTURE UPLOADED

=> Uploading C:\STNEXP4\QUERIES\aw9.str

L18 STRUCTURE UPLOADED

=> s 117 SAMPLE SEARCH INITIATED 10:25:29 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 4837 TO ITERATE

20.7% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 92570 TO 100910 PROJECTED ANSWERS: 0 TO 0

L19 0 SEA SSS SAM L17

=> search 117
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 10:25:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 96489 TO ITERATE

100.0% PROCESSED 96489 ITERATIONS SEARCH TIME: 00.00.15

0 ANSWERS

L20 0 SEA SSS FUL L17

=> s 118

SAMPLE SEARCH INITIATED 10:26:01 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 10214 TO ITERATE

9.8% PROCESSED 1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

198224 TO 210336

PROJECTED ANSWERS:

0 TO 0

T.21

0 SEA SSS SAM L18

=> search 118

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.

ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET: full

FULL SEARCH INITIATED 10:26:14 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 203759 TO ITERATE

100.0% PROCESSED 203759 ITERATIONS

21 ANSWERS

-

SEARCH TIME: 00.00.14

L22 21 SEA SSS FUL L18

=>

Uploading C:\STNEXP4\QUERIES\all.str

L23 STRUCTURE UPLOADED

=> d 123

L23 HAS NO ANSWERS

L23

STF

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 123

SAMPLE SEARCH INITIATED 10:32:40 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 177 TO ITERATE

100.0% PROCESSED 177 ITERATIONS (19 INCOMPLETE) 19 ANSWERS

SEARCH TIME: 00.00.03

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

2742 TO 4338

PROJECTED ANSWERS:

119 TO 641

L24

19 SEA SSS SAM L23

=> s 123

SAMPLE SEARCH INITIATED 10:32:50 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 177 TO ITERATE

100.0% PROCESSED 177 ITERATIONS (19 INCOMPLETE) 19 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 2742 TO 4338 PROJECTED ANSWERS: 119 TO 641

L25 19 SEA SSS SAM L23

=> search 123

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 10:33:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3334 TO ITERATE

100.0% PROCESSED 3334 ITERATIONS (300 INCOMPLETE) 300 ANSWERS SEARCH TIME: 00.00.11

L26 300 SEA SSS FUL L23

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 838.04 846.23

FILE 'CAPLUS' ENTERED AT 10:33:22 ON 24 JAN 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 24 Jan 2005 VOL 142 ISS 5 FILE LAST UPDATED: 23 Jan 2005 (20050123/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 126

L27 123 L26

=> d 127 fbib ab hitstr 1-123

L27 ANSWER 1 OF 123 CAPLUS COPYRIGHT 2005 ACS on STN

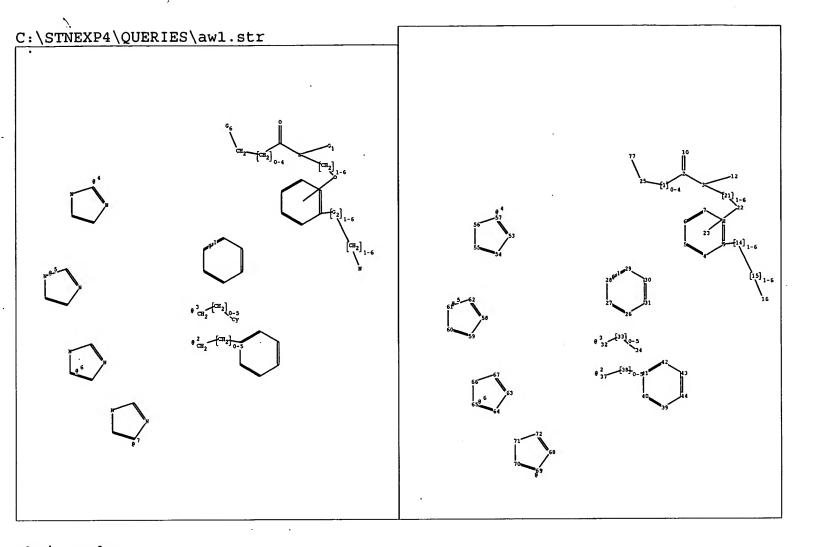
AN 2004:1059377 CAPLUS

DN 142:19573

TI Purification means

IN Hay, Alastair; Cotton, Graham; Ramage, Robert

PA CSS-Albachem Limited, UK



chain nodes : 38 1 2 3 10 12 14 15 16 21 22 25 32 33 34 37 77 ring nodes : 8 9 26 27 28 29 30 31 39 40 41 42 43 44 4 5 6 7 66 67 68 69 70 71 55 56 57 58 59 60 61 62 63 64 65 chain bonds : 1-2 1-25 2-3 2-10 3-12 3-21 9-14 14-15 15-16 21-22 25-77 32-33 33-34 37-38 38-41 ring bonds : 4-5 4-9 5-6 6-7 7-8 8-9 26-27 26-31 27-28 28-29 29-30 30-31 42-43 43-44 53-54 53-57 54-55 55-56 .39-40 39-44 40-41 41-42 61-62 63-64 63-67 64-65 59-60 60-61 65-66 56-57 58-59 58-62 71-72 69-70 70-71 66-67 68-69 68-72 exact/norm bonds : 9-14 14-15 25-77 33-34 53-54 53-57 54-55 55-56 2-3 2-10 3-12 60-61 61-62 63-64 63-67 64-65 65-66 56-57 58-59 58-62 59-60 71-72 66-67 68-69 68-72 69-70 70-71 exact bonds : 1-2 1-25 3-21 15-16 21-22 32-33 37-38 38-41

4-5 4-9 5-6 6-7 7-8 8-9 26-27 26-31 39-40 39-44 40-41 41-42 42-43 43-44

27-28 28-29 29-30 30-31

G1:H,Ak

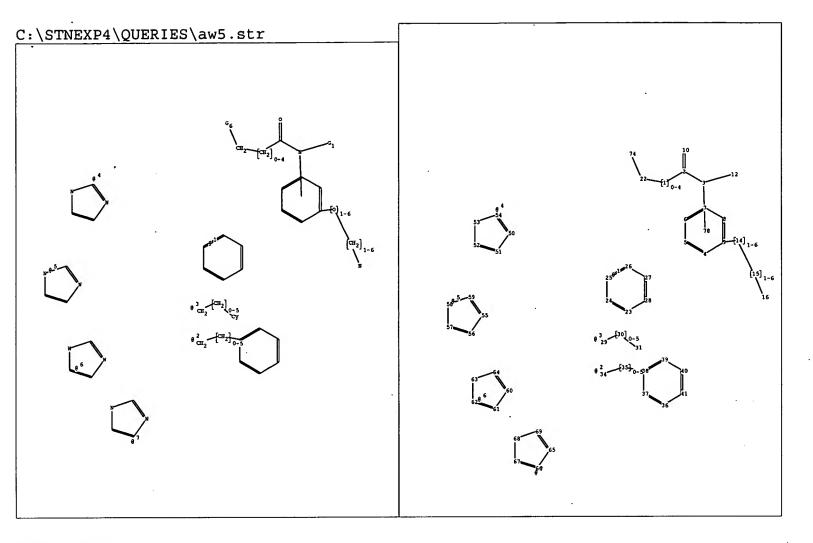
normalized bonds :

G2:0, N, C

G3:0, CH2

```
G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]
G5:CH3, Et, n-Pr, i-Pr, i-Bu, s-Bu, t-Bu, [*1], [*3]
G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]
Match level :
                              4:Atom 5:Atom 6:Atom 7:Atom
                                                              8:Atom 9:Atom
    1:CLASS
            2:CLASS
                     3:CLASS
                       14:CLASS 15:CLASS
                                           16:CLASS
                                                     21:CLASS
                                                               22:CLASS
    10:CLASS
             12:CLASS
                                         28:Atom 29:Atom 30:Atom 31:Atom
                       26:Atom
                                27:Atom
    23:CLASS
             25:CLASS
                                          38:CLASS 39:Atom 40:Atom
                                37:CLASS
    32:CLASS
             33:CLASS
                       34:Atom
    41:Atom 42:Atom 43:Atom
                             44:Atom 53:Atom 54:Atom
                                                        55:Atom
                                                                  56:Atom
                                                62:Atom
                                                         63:Atom
                                                                  64:Atom
    57:Atom
            58:Atom
                     59:Atom
                              60:Atom
                                       61:Atom
    65:Atom 66:Atom 67:Atom
                             68:Atom
                                       69:Atom
                                                70:Atom
                                                         71:Atom
                                                                  72:Atom
```

77:CLASS



chain nodes : 30 31 35 74 14 15 16 22 29 34 1 2 3 10 12 ring nodes : 24 25 26 27 28 36 37 38 39 40 41 50 51 4 5 6 7 8 9 23 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 chain bonds : 1-2 1-22 2-3 2-10 3-12 9-14 14-15 15-16 22-74 29-30 30-31 34-35 35-38 ring bonds : 5-6 6-7 7-8 8-9 23-24 23-28 24-25 25-26 26-27 27-28 4-5 4-9 36-37 36-41 37-38 38-39 39-40 40-41 50-51 50-54 51-52 52-53 58-59 60-61 60-64 61-62 62-63 53-54 55-56 55-59 56-57 57-58 63-64 65-66 66-67 67-68 68-69 65-69 exact/norm bonds : 9-14 22-74 30-31 50-51 50-54 51-52 52-53 53-54 2-3 2-10 3-12 55-56 55-59 56-57 57-58 58-59 60-61 60-64 61-62 62-63 63-64 65-66 65-69 66-67 67-68 68-69 exact bonds : 1-2 1-22 14-15 15-16 29-30 34-35 35-38

normalized bonds :

4-5 4-9 5-6 6-7 7-8 8-9 23-24 23-28 24-25 25-26 26-27 27-28 36-37 36-41 37-38 38-39 39-40 40-41

G1:H,Ak

G2:0,N,C

G3:0, CH2

```
G5:CH3, Et, n-Pr, i-Pr, i-Bu, s-Bu, t-Bu, [*1], [*3]
G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]
Match level :
                                                              8:Atom 9:Atom
                               4:Atom
                                      5:Atom 6:Atom 7:Atom
    1:CLASS
             2:CLASS
                      3:CLASS
                                                     22:CLASS
                                                                23:Atom
                        14:CLASS 15:CLASS
                                            16:CLASS
    10:CLASS
              12:CLASS
                                                 29:CLASS
                                                           30:CLASS
                               27:Atom
                                        28:Atom
    24:Atom
             25:Atom
                      26:Atom
                                                                     41:Atom
                        36:Atom 37:Atom 38:Atom 39:Atom 40:Atom
    34:CLASS
              35:CLASS
                              53:Atom 54:Atom 55:Atom 56:Atom 57:Atom
            51:Atom
                     52:Atom
    50:Atom
                                                         64:Atom
                                        62:Atom
                                                 63:Atom
    58:Atom
             59:Atom
                     60:Atom
                               61:Atom
```

74:CLASS

78:CLASS

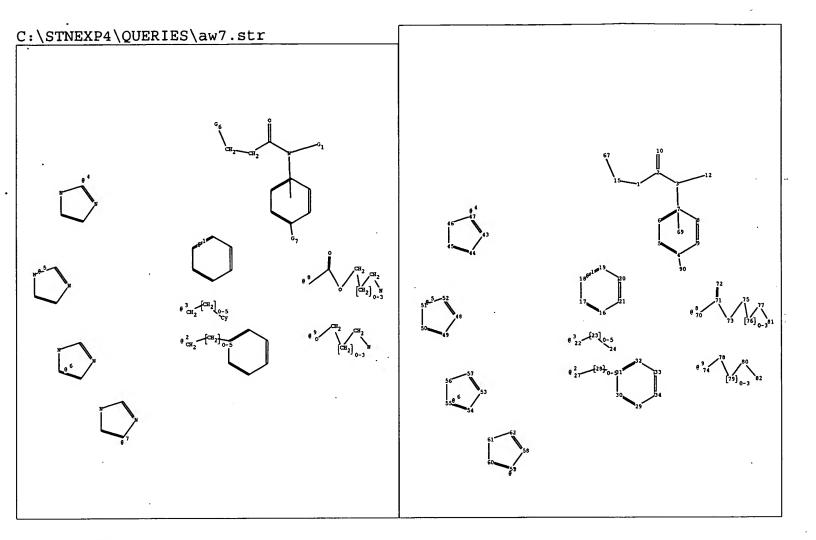
69:Atom

G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]

68:Atom

67:Atom

66:Atom

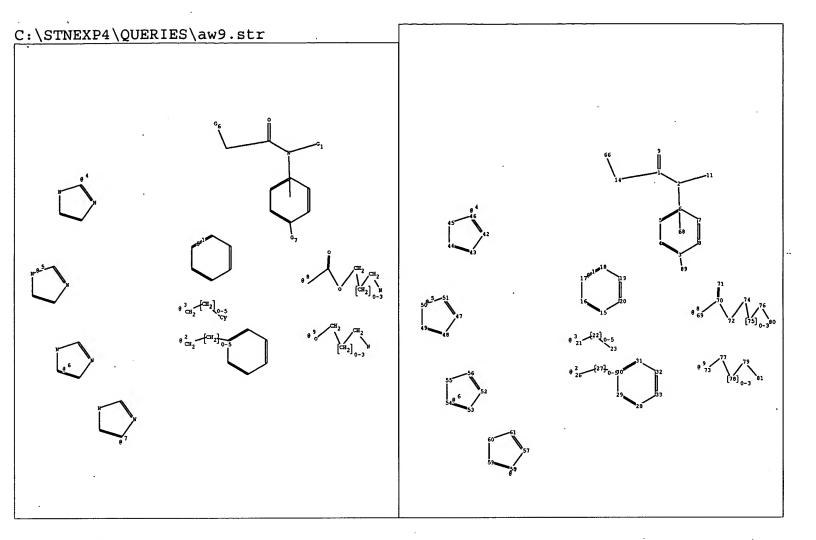


1 2 3 10 12 15 22 23 24 27 67 70 71 72 73 74 75 76 28 77 78 79 80 81 82 90 ring nodes : 4 5 6 7 8 9 16 17 18 19 20 21 29 30 31 32 33 34 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 chain bonds : 4-90 15-67 22-23 23-24 27-28 28-31 1-2 1-15 2-3 2-10 3-12 70-71 71-72 71-73 73-75 74-78 75-76 76-77 77-81 78-79 79-80 80-82 ring bonds : 5-6 6-7 7-8 8-9 16-17 16-21 17-18 18-19 19-20 20-21 4-5 4-9 29-30 29-34 30-31 31-32 32-33 33-34 43-44 43-47 44-45 45-46 54-55 51-52 53-54 53-57 46-47 48-49 48-52 49-50 50-51 56-57 58-59 58-62 59-60 60-61 61-62 exact/norm bonds : 2-3 2-10 3-12 4-90 15-67 23-24 43-44 43-47 44-45 45-46 46-47 48-49 48-52 49-50 50-51 51-52 53-54 53-57 54-55 55-56 56-57 58-59 58-62 59-60 60-61 61-62 71-72 71-73 exact bonds : 1-2 1-15 22-23 27-28 28-31 70-71 73-75 74-78 75-76 76-77 77-81 78-79 79-80 80-82 normalized bonds : 4-5 4-9 5-6 6-7 7-8 8-9 16-17 16-21 17-18 18-19 19-20 20-21

29-30 29-34 30-31 31-32 32-33 33-34

```
G3:0,CH2
G4:H, CH3, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, [*1], [*2]
G5:CH3, Et, n-Pr, i-Pr, i-Bu, s-Bu, t-Bu, [*1], [*3]
G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]
G7: [*8], [*9]
Match level:
    1:CLASS
             2:CLASS
                      3:CLASS
                               4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
                                 16:Atom 17:Atom
                                                    18:Atom
                                                             19:Atom
                                                                      20:Atom
                        15:CLASS
    10:CLASS
              12:CLASS
                                 24:Atom 27:CLASS
                                                    28:CLASS
                                                              29:Atom
                       23:CLASS
    21:Atom 22:CLASS
             31:Atom
                                        34:Atom
                                                43:Atom
                                                         44:Atom
    30:Atom
                      32:Atom
                               33:Atom
                                                                   53:Atom
                              49:Atom
                                        50:Atom
                                                 51:Atom
                                                          52:Atom
    46:Atom
             47:Atom
                      48:Atom
             55:Atom
                      56:Atom
                               59:Atom
                                                          60:Atom
                                                                   61:Atom
    54:Atom
                                           71:CLASS
                                                     72:CLASS
                                                               73:CLASS
                       69:CLASS
                                 70:CLASS
    62:Atom 67:CLASS
                        76:CLASS
                                  77:CLASS
                                            78:CLASS
                                                     79:CLASS
                                                                80:CLASS
              75:CLASS
    74:CLASS
    81:CLASS
              82:CLASS
                        90:CLASS
```

G2:0,N,C



23 26 27 66 69 70 71 72 73 74 75 76 1 2 9 11 14 21 22 77 78 79 80 81 89 ring nodes : 7 8 15 16 17 18 19 20 28 29 30 31 32 3 4 5 6 33 42 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 44 45 46 chain bonds : 22-23 1-9 1-2 1-14 2-11 3-89 14-66 21-22 26-27 27 - 3069-70 70-71 70-72 72-74 73-77 74-75 75-76 76-80 77-78 78-79 79-81 ring bonds : 6-7 7-8 15-16 15-20 16-17 17-18 3-4 3-8 4-5 5-6 18-19 19-20 29-30 30-31 31-32 32-33 42-43 42-46 43-44 44-45 28-29 28-33 50-51 52-53 52-56 53-54 54-55 45-46 47-48 47-51 48-49 49-50 55-56 57-58 57-61 58-59 59-60 60-61 exact/norm bonds : 42-43 42-46 43-44 44-45 45-46 1-9 1-2 2-11 3-89 14-66 22-23 47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55 55-56 57-58 57-61 58-59 59-60 60-61 70-71 70 - 72exact bonds : 1-14 21-22 26-27 27-30 69-70 72-74 73-77 74-75 75-76 76-80 77-78 78-79 79-81 normalized bonds :

16-17

17-18

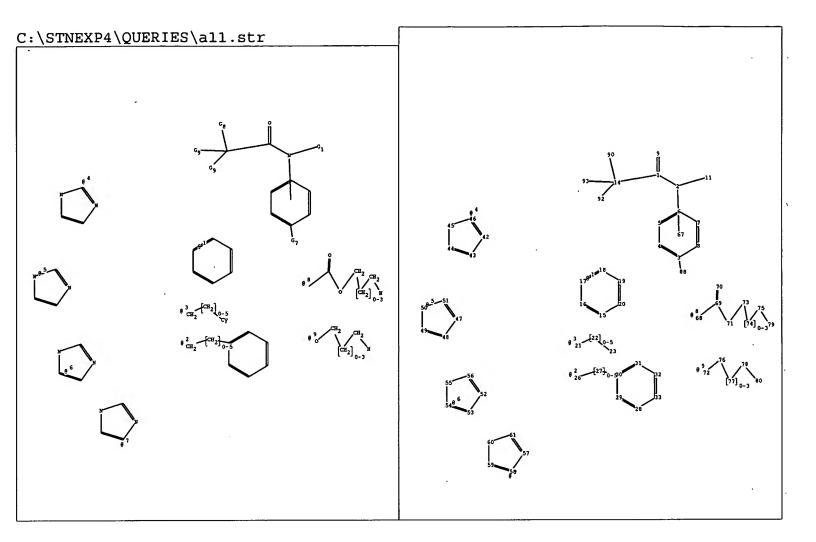
18-19

3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20

28-29 28-33 29-30 30-31 31-32 32-33

```
G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]
G5:CH3, Et, n-Pr, i-Pr, i-Bu, s-Bu, t-Bu, [*1], [*3]
G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]
G7: [*8], [*9]
Match level:
    1:CLASS
             2:CLASS
                      3:Atom 4:Atom 5:Atom 6:Atom
                                                      7:Atom
                                                              8:Atom
                                 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
    11:CLASS
              14:CLASS
                        15:Atom
              22:CLASS
                        23:Atom
                                 26:CLASS
                                           27:CLASS
                                                     28:Atom 29:Atom
    21:CLASS
    30:Atom · 31:Atom 32:Atom 33:Atom 42:Atom 43:Atom 44:Atom 45:Atom
                                        50:Atom 51:Atom
                                                         52:Atom
                                                                   53:Atom
                     48:Atom
                              49:Atom
    46:Atom
             47:Atom
                                                          60:Atom
                                        58:Atom 59:Atom
                                                                   61:Atom
    54:Atom
             55:Atom
                     56:Atom
                               57:Atom
                        69:CLASS
                                  70:CLASS
                                            71:CLASS
                                                      72:CLASS
                                                                73:CLASS
    66:CLASS
              68:CLASS
              75:CLASS
                        76:CLASS
                                  77:CLASS
                                            78:CLASS
                                                      79:CLASS
                                                                80:CLASS
    74:CLASS
    81:CLASS
              89:CLASS
```

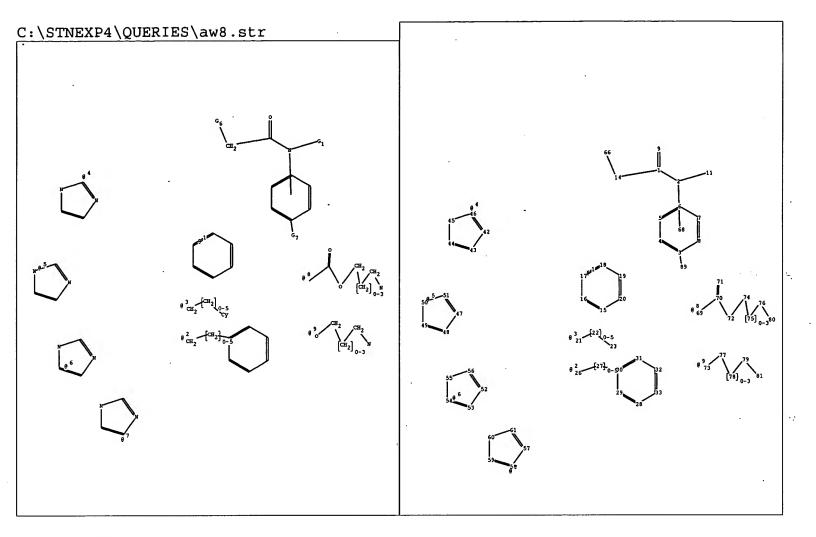
G3:0,CH2



```
1 2 9 11 14 21 22 23 26
                                27
                                    68
                                        69
                                           70
                                               71
                                                  72
                                                      73
                                                          74
                                                             75
                                                                 76
   77 78 79 80 88 90 92
                           93
ring nodes :
              7 8 15 16 17 18 19 20 28 29 30 31 32 33 42 43
   3 4 5 6
   44 45 46 47 48 49 50 51 52 53 54
                                         55 56
                                                 57
                                                    58
                                                       59 60 61
chain bonds :
                            14-90
                                  14-92
                                        14-93
   1-9 1-2 1-14 2-11 3-88
                                               21-22
                                                     22-23
                                                           26-27
   27-30 68-69 69-70 69-71 71-73 72-76 73-74 74-75
                                                           76-77
                                                     75-79
   77-78 78-80
ring bonds :
   3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
   28-29 28-33 29-30 30-31 31-32 32-33 42-43 42-46 43-44 44-45
                                  50-51 52-53 52-56
                                                     53-54
                                                           54-55
                     48-49
                            49-50
   45-46 47-48 47-51
   55-56 57-58 57-61
                      58-59
                            59-60
                                  60-61
exact/norm bonds :
                                  14-93
                                         22-23 42-43 42-46 43-44
   1-9 1-2 2-11 3-88
                      14-90 14-92
   44-45 45-46 47-48 47-51 48-49
                                  49-50
                                        50-51 52-53
                                                    52-56 53-54
   54-55 55-56 57-58 57-61 58-59
                                  59-60 60-61 69-70
                                                    69-71
exact bonds :
   1-14 21-22
               26-27
                     27-30 68-69 71-73 72-76 73-74 74-75
                                                          75-79
   76-77 77-78 78-80
normalized bonds :
   3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20
                                          16-17 17-18 18-19 19-20
```

28-29 28-33 29-30 30-31 31-32 32-33

```
G2:0, N, C
G3:0, CH2
G4:H, CH3, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, [*1], [*2]
G5:CH3, Et, n-Pr, i-Pr, i-Bu, s-Bu, t-Bu, [*1], [*3]
G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]
G7: [*8], [*9]
G8:CH3, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, [*1]
G9:H, CH3, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, [*1]
Match level :
                       3:Atom 4:Atom 5:Atom 6:Atom
                                                        7:Atom
                                                                 8:Atom
                                                                         9:CLASS
    1:CLASS
             2:CLASS
                                  16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
              14:CLASS
                         15:Atom
    11:CLASS
                                   26:CLASS 27:CLASS
                                                        28:Atom 29:Atom
              22:CLASS
                         23:Atom
    21:CLASS
                                33:Atom 42:Atom
                                                   43:Atom
                                                            44:Atom
                                                                      45:Atom
    30:Atom
             31:Atom
                      32:Atom
    46:Atom
             47:Atom
                       48:Atom
                                49:Atom
                                         50:Atom
                                                   51:Atom
                                                             52:Atom
                                                                       53:Atom
                                57:Atom
                                          58:Atom
                                                   59:Atom
                                                             60:Atom
                                                                       61:Atom
             55:Atom
                       56:Atom
    54:Atom
                                    70:CLASS
                                              71:CLASS
                                                         72:CLASS
                                                                   73:CLASS
              68:CLASS
                         69:CLASS
    67:CLASS
                                                         79:CLASS
                                              78:CLASS
                                                                   80:CLASS
                         76:CLASS
                                    77:CLASS
    74:CLASS
              75:CLASS
    88:CLASS
              90:CLASS
                         92:CLASS
                                    93:CLASS
```



1 2 9 11 14 21 22 77 78 79 80 81 89 ring nodes : 3 4 5 6 7 8 15 16 17 18 19 20 28 29 30 31 32 33 42 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 chain bonds : 22-23 26-27 69-70 1-9 1-2 1-14 2-11 3-89 14-66 21-22 27-30 75-76 76-80 77-78 78 - 7970-71 70-72 72-74 73-77 74-75 79-81 ring bonds : 6-7 7-8 15-16 15-20 16-17 17-18 18-19 3-4 3-8 4-5 5-6 28-29 28-33 29-30 31-32 32-33 42-43 42-46 43-44 44-45 30-31 45-46 47-48 47-51 49-50 50-51 52-53 52-56 53-54 54-55 48-49 55-56 57-58 57-61 58-59 59-60 60-61 exact/norm bonds : 1-9 1-2 2-11 3-89 14-66 22-23 42-43 42-46 43-44 44-45 45-46 52-56 53-54 54-55 55-56 47-48 47-51 48-49 49-50 50-51 52-53 57-58 57-61 58-59 70-71 70-72 59-60 60-61 exact bonds : 1-14 21-22 26-27 27-30 69-70 72-74 73-77 74-75 75-76 76-80 77-78 78-79 79-81 normalized bonds : 3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20

27

66

69

70

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72

73

74

75

76

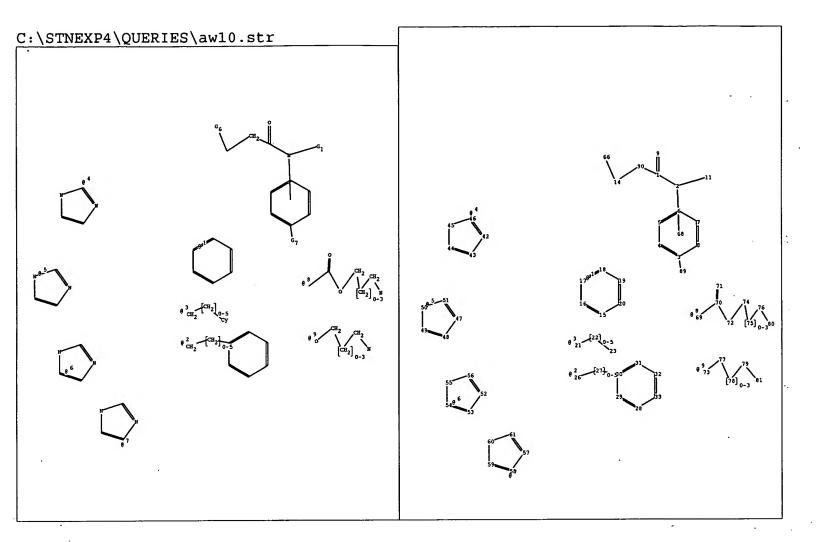
23

28-29 28-33 29-30 30-31 31-32 32-33

26

```
G4:H, CH3, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, [*1], [*2]
G5:CH3, Et, n-Pr, i-Pr, i-Bu, s-Bu, t-Bu, [*1], [*3]
G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]
G7:[*8],[*9]
Match level :
                                                       7:Atom
                                                                8:Atom 9:CLASS
    1:CLASS
             2:CLASS
                      3:Atom 4:Atom 5:Atom 6:Atom
                                  16:Atom 17:Atom 18:Atom
                                                             19:Atom 20:Atom
    11:CLASS
              14:CLASS
                        15:Atom
                         23:Atom
                                  26:CLASS
                                            27:CLASS
                                                      28:Atom 29:Atom
    21:CLASS
              22:CLASS
                               33:Atom 42:Atom 43:Atom 44:Atom 45:Atom
    30:Atom
             31:Atom
                     32:Atom
                                                  51:Atom
                                                           52:Atom
                                49:Atom
                                         50:Atom
                                                                     53:Atom
             47:Atom
                      48:Atom
    46:Atom
                                57:Atom
                                                  59:Atom
                                                            60:Atom
    54:Atom
             55:Atom
                      56:Atom
                                         58:Atom
                                             71:CLASS
                                                       72:CLASS
                                                                  73:CLASS
    66:CLASS
              68:CLASS
                         69:CLASS
                                   70:CLASS
                         76:CLASS
                                   77:CLASS
                                             78:CLASS
                                                       79:CLASS
                                                                  80:CLASS
    74:CLASS
              75:CLASS
    81:CLASS
              89:CLASS
```

G3:0,CH2



```
1 2 9 11 14 21 22 23
                             26
                                 27
                                     66
                                        69
                                           70
                                                71
                                                   72
                                                       73
                                                          74 75 . 76
   77 78 79
              80 81 89 90
ring nodes :
              7 8 15 16 17 18 19 20 28 29 30 31 32 33 42 43
   3 4 5 6
   44 45 46
              47 48 49 50
                            51 52
                                   53 54 55 56
                                                 57
                                                     58 59 60 61
chain bonds :
   1-9 1-2 1-90 2-11 3-89
                            14-66
                                   14-90
                                         21-22
                                                22-23
                                                      26-27
                                                            27 - 30
   69-70 70-71 70-72 72-74 73-77 74-75
                                               76-80
                                                     77-78
                                                            78 - 79
                                        75-76
   79-81
ring bonds :
           4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
   3-4 3-8
   28-29 28-33 29-30 30-31 31-32 32-33 42-43 42-46 43-44 44-45
                      48-49 49-50
                                  50-51
                                         52-53 52-56
                                                     53-54
   45-46 47-48
               47-51
                                   60-61
   55-56 57-58
                57-61
                      58-59
                            59-60
exact/norm bonds :
                                         42-46 43-44 44-45 45-46
                            22-23
                                   42-43
   1-9 1-2 2-11 3-89
                      14-66
                                  52-53 52-56 53-54 54-55 55-56
   47-48 47-51 48-49 49-50
                            50-51
   57-58 57-61 58-59 59-60
                            60-61
                                   70-71
                                         70-72
exact bonds :
                     26-27 27-30 69-70 72-74 73-77 74-75
                                                           75-76
   1-90
        14-90 21-22
   76-80 77-78
               78-79 79-81
normalized bonds :
   3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20
                                           16-17
                                                 17-18
                                                        18-19 19-20
```

28-29 28-33 29-30 30-31 31-32 32-33

```
G3:0, CH2
G4:H, CH3, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, [*1], [*2]
G5:CH3, Et, n-Pr, i-Pr, i-Bu, s-Bu, t-Bu, [*1], [*3]
G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]
G7: [*8], [*9]
Match level:
                      3:Atom 4:Atom 5:Atom 6:Atom
                                                      7:Atom
                                                               8:Atom
    1:CLASS
             2:CLASS
                        15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
                                                                      20:Atom
    11:CLASS
              14:CLASS
                                                      28:Atom 29:Atom
                        23:Atom 26:CLASS 27:CLASS
              22:CLASS
    21:CLASS
                               33:Atom 42:Atom 43:Atom
    30:Atom 31:Atom
                                                          44:Atom
                      32:Atom
                                        50:Atom
                                                 51:Atom
                                                           52:Atom
                                                                    53:Atom
    46:Atom
             47:Atom
                      48:Atom
                               49:Atom
                      56:Atom
                               57:Atom
                                        58:Atom 59:Atom
                                                           60:Atom
                                                                    61:Atom
    54:Atom
             55:Atom
              68:CLASS
                                            71:CLASS
                                                       72:CLASS
                                                                 73:CLASS
                        69:CLASS
                                  70:CLASS
    66:CLASS
                                  77:CLASS
                                            78:CLASS
                                                       79:CLASS
                                                                 80:CLASS
              75:CLASS
                        76:CLASS
    74:CLASS
    81:CLASS
              89:CLASS 90:CLASS
```

G2:0, N, C